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Structural changes of silicagel by compression

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The structural changes of silica gel by compression
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The structural change in amorphous silica gel ($SiO_2 nH_2O$) compressed up to about 1GPa and investigated by X-ray diffraction, Raman and Infrared spectroscopic measurements for elucidate the structural change processes.

Silica gel powder put in an Al alloy tube and compressed with 25kN to 200kN of press loads. Observed X-ray diffraction patterns show typical halo patterns for amolphous materials which have maxima at about 2theta=23degree (FSDP). FSDP shifted to higher angle by compression. Tan and Arndt (1999, J. Non-Cryst., Solids, 82, 117) reported that the shift of FSDP position to higher angle for compressed SiO_2 glass and this caused by decreasing in size of intermediate-range order of silica glass to increase its density.

In Raman spectrum, the 430 cm^{-1} broad band attributed to Si-O-Si symmetric stretching vibrations became sharp and the average position shifts to high wavenumber by compression. This shows that Si-O-Si angle in SiO4 tetrahedral linkage in SiO4-X(OH)x decrease. The new band appears at 600cm^{-1} in 50 kN and the intensity increase in increasing of compression load. This band has been attributed to three-membered rings of SiO_4 tetrahedra. The intensity of 980cm^{-1} band of silanol groups increases by compression. This fact shows that some silanorl groups reacts to dehydrate and form three-membered rings of SiO_4 tetrahedra. However, this dehydration reaction are limited and most H_2O and silanol groups were remained. Because, Raman band around 3500cm^{-1} associate with H_2O almost remains its intensity after compression.

In IR spectra, the intensity of 800cm^{-1} band of Si-O-Si bending mode increased by compression. It is consistent with formation of three-membered rings of SiO_4 tetrahedra those were found in Raman study. The FWHM of the 1080cm^{-1} band increases and the band position shifts to lower wavenumber by compression. These facts show that the deformation of SiO_4 tetrahedron and the average Si-O length increase by compression.